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\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	3	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	4	AUG 13	CA/CAPplus enhanced with additional kind codes for granted patents
NEWS	5	AUG 20	CA/CAPplus enhanced with CAS indexing in pre-1907 records
NEWS	6	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	7	AUG 27	USPATOLD now available on STN
NEWS	8	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS	9	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS	10	SEP 13	FORIS renamed to SOFIS
NEWS	11	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	12	SEP 17	CA/CAPplus enhanced with printed CA page images from 1967-1998
NEWS	13	SEP 17	CAPplus coverage extended to include traditional medicine patents
NEWS	14	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	15	OCT 02	CA/CAPplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	16	OCT 19	BEILSTEIN updated with new compounds
NEWS	17	NOV 15	Derwent Indian patent publication number format enhanced
NEWS	18	NOV 19	WPIX enhanced with XML display format
NEWS	19	NOV 30	ICSD reloaded with enhancements
NEWS	20	DEC 04	LINPADOCDB now available on STN
NEWS	21	DEC 14	BEILSTEIN pricing structure to change
NEWS	22	DEC 17	USPATOLD added to additional database clusters
NEWS	23	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS	24	DEC 17	DGENE now includes more than 10 million sequences
NEWS	25	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS	26	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS	27	DEC 17	CA/CAPplus enhanced with new custom IPC display formats
NEWS	28	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS	29	JAN 02	STN pricing information for 2008 now available
NEWS	30	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	31	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	32	JAN 28	MARPAT searching enhanced

NEWS 33 JAN 28 USGENE now provides USPTO sequence data within 3 days  
of publication

NEWS 34 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment

NEWS 35 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS LOGIN Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that  
specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 11:52:01 ON 01 FEB 2008

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:52:06 ON 01 FEB 2008

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STRUCTURE FILE UPDATES: 31 JAN 2008 HIGHEST RN 1001228-41-6

DICTIONARY FILE UPDATES: 31 JAN 2008 HIGHEST RN 1001228-41-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when  
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REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> file casreact

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.46	0.67

FILE 'CASREACT' ENTERED AT 11:52:10 ON 01 FEB 2008  
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FILE CONTENT:1840 - 26 Jan 2008 VOL 148 ISS 5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

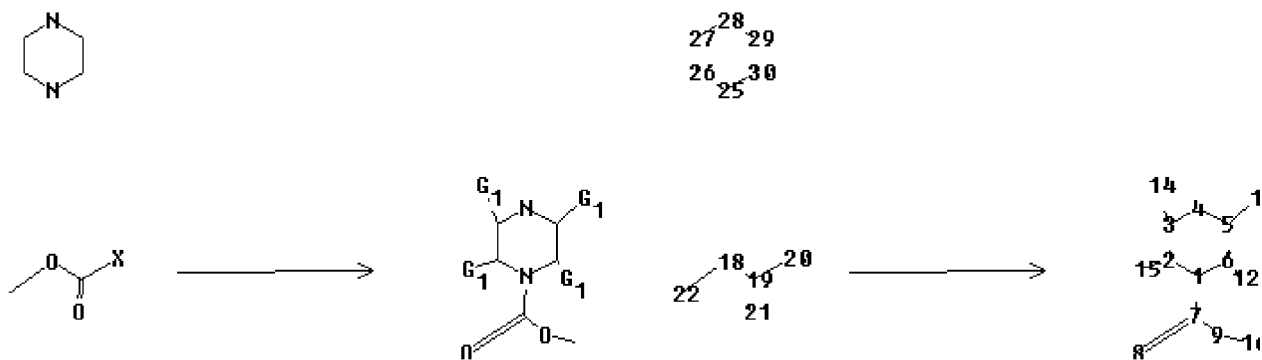
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*****
*
*      CASREACT now has more than 13.8 million reactions
*
*****
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Program Files\Stnexp\Queries\10524517form3rxn.str



chain nodes :

7 8 9 11 12 14 15 18 19 20 21

ring nodes :

1 2 3 4 5 6 25 26 27 28 29 30

ring/chain nodes :

16 22

chain bonds :

1-7 2-15 3-14 5-11 6-12 7-8 7-9 9-16 18-19 18-22 19-20 19-21

ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 25-26 25-30 26-27 27-28 28-29 29-30  
 exact/norm bonds :  
 1-2 1-6 1-7 2-3 2-15 3-4 3-14 4-5 5-6 5-11 6-12 7-8 7-9 9-16 18-19  
 18-22 19-21 25-26 25-30 26-27 27-28 28-29 29-30  
 exact bonds :  
 19-20  
 isolated ring systems :  
 containing 1 :

G1:C,H,O,X

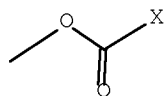
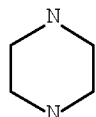
Match level :  
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 12:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS  
 22:CLASS 25:Atom  
 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom  
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 containing 18  
 fragments assigned reagent role:  
 containing 25  
 fragments assigned product role:  
 containing 1

L1 STRUCTURE UPLOADED

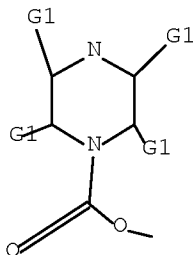
=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,H,O,X



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

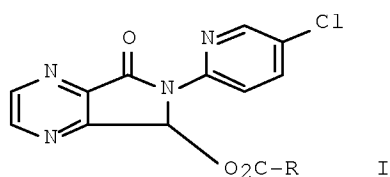
FULL SEARCH INITIATED 11:52:35 FILE 'CASREACT'  
SCREENING COMPLETE - 113 REACTIONS TO VERIFY FROM 11 DOCUMENTS  
100.0% DONE 113 VERIFIED 9 HIT RXNS 2 DOCS  
SEARCH TIME: 00.00.01

L2 2 SEA SSS FUL L1 ( 9 REACTIONS)

=> d ibib abs hit

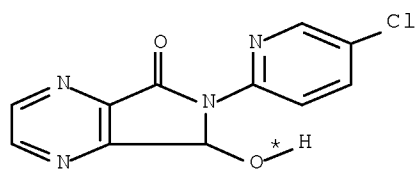
L2 ANSWER 1 OF 2 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 143:211927 CASREACT Full-text  
TITLE: Preparation of optically active carbonate  
intermediates in synthesis of (+)-zopiclone  
INVENTOR(S): Bayod Jasanada, Miguel; Sanchez Pedregal, Victor M.;  
Gotor Santamaria, Vicente; Brieva Collado, M. Rosario;  
Fernandez Solares, Laura; Diaz Sierra, Monica; Guisan  
Seijas, Jose Manuel; Paloma Carmona, Jose Miguel;  
Fernandez-Lafuente, Roberto  
PATENT ASSIGNEE(S): Universidad de Oviedo, Spain; Astur Pharma, S.A.  
SOURCE: Span., 12 pp.  
CODEN: SPXXAD  
DOCUMENT TYPE: Patent  
LANGUAGE: Spanish  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ES 2203319	A1	20040401	ES 2002-771	20020403
ES 2203319	B1	20050301		
US 6969767	B1	20051129	US 2003-405998	20030402
PRIORITY APPLN. INFO.:			ES 2002-771	20020403
OTHER SOURCE(S):	MARPAT 143:211927			
GI				

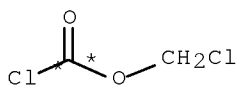


AB The invention relates to the synthesis of carbonates I (R = isopropenyloxy, p-nitrophenoxy, chloromethoxy, 1-chloro-, 2-chloro-, 2,2,2-trichloro- or 1,1-dimethyl-2,2,2-trichloroethoxy), their resolution, and use in the synthesis of (+)-zopiclone [(S)-I; R = 4-methyl-1-piperazinyl]. Thus, (S)-I (R = ClCH<sub>2</sub>O) was prepared by esterification of 6-(5-chloro-2-pyridinyl)-5-hydroxy-7-oxo-5,6-dihydropyrrolo[3,4-b]pyrazine with p-nitrophenyl chloroformate and resolution using immobilized lipase B from *Candida antarctica*. Treatment of the product with N-methylpiperazine afforded (+)-zopiclone.

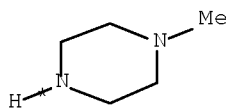
RX(14) OF 14 COMPOSED OF RX(7), RX(9), RX(8)  
 RX(14) A + P + R ==> T



A

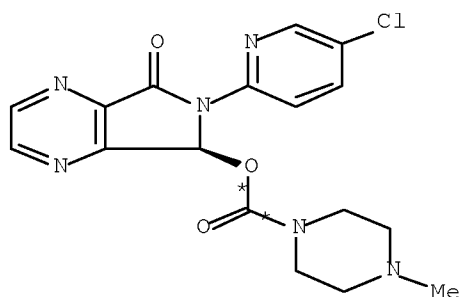


P



R

3  
 STEPS



T  
 YIELD 90%

RX(7) RCT A 43200-81-3, P 22128-62-7  
 RGT D 110-86-1 Pyridine  
 PRO Q 508169-18-4  
 SOL 75-09-2 CH2Cl2  
 CON SUBSTAGE(1) 0 deg C  
 SUBSTAGE(2) 17 hours, room temperature

RX(9) RCT Q 508169-18-4  
 RGT V 290-37-9 Pyrazine  
 PRO S 508169-20-8  
 CAT 9001-62-1 Lipase  
 SOL 7732-18-5 Water, 108-88-3 PhMe  
 CON 100 hours, 60 deg C, pH 7

NTE biotransformation, enzymic(immobilized lipase B from Candida antarctica used), buffered solution(phosphate), stereoselective

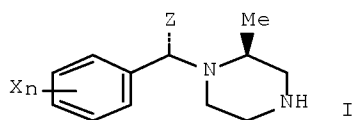
RX(8) RCT R 109-01-3, S 508169-20-8  
PRO T 138729-47-2  
SOL 67-64-1 Me2CO  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 2 hours, 0 deg C -> 15 deg C

=> d 12 ibib abs hit 2

L2 ANSWER 2 OF 2 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 139:307801 CASREACT Full-text  
TITLE: Stereoselective alkylation of chiral  
2-methyl-4-protected piperazines  
INVENTOR(S): Wu, Wenxue; Liao, Hongbiao; Tsai, David J.; Andrews,  
David R.; Gala, Dinesh; Lee, Gary M.; Schwartz, Martin  
Lawrence; McAllister, Timothy L.; Fu, Xiaoyong;  
Maloney, Donal; Thiruvengadam, T. K.; Tann, Chou-Hang  
PATENT ASSIGNEE(S): Schering Corporation, USA  
SOURCE: PCT Int. Appl., 39 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2003084942	A2	20031016	WO 2003-US9275	20030327
WO 2003084942	A3	20040506		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2480481	A1	20031016	CA 2003-2480481	20030327
AU 2003239128	A1	20031020	AU 2003-239128	20030327
US 2003208074	A1	20031106	US 2003-400429	20030327
US 6872826	B2	20050329		
EP 1490346	A2	20041229	EP 2003-733842	20030327
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
CN 1642930	A	20050720	CN 2003-807388	20030327
JP 2005526826	T	20050908	JP 2003-582139	20030327
CN 101092401	A	20071226	CN 2007-10140725	20030327
ZA 2004006469	A	20050920	ZA 2004-6469	20040813
MX 2004PA09414	A	20050125	MX 2004-PA9414	20040928
US 2005171120	A1	20050804	US 2005-89858	20050325
PRIORITY APPLN. INFO.:			US 2002-368707P	20020329
			CN 2003-807388	20030327
			US 2003-400429	20030327
			WO 2003-US9275	20030327
OTHER SOURCE(S):	MARPAT 139:307801			

GI

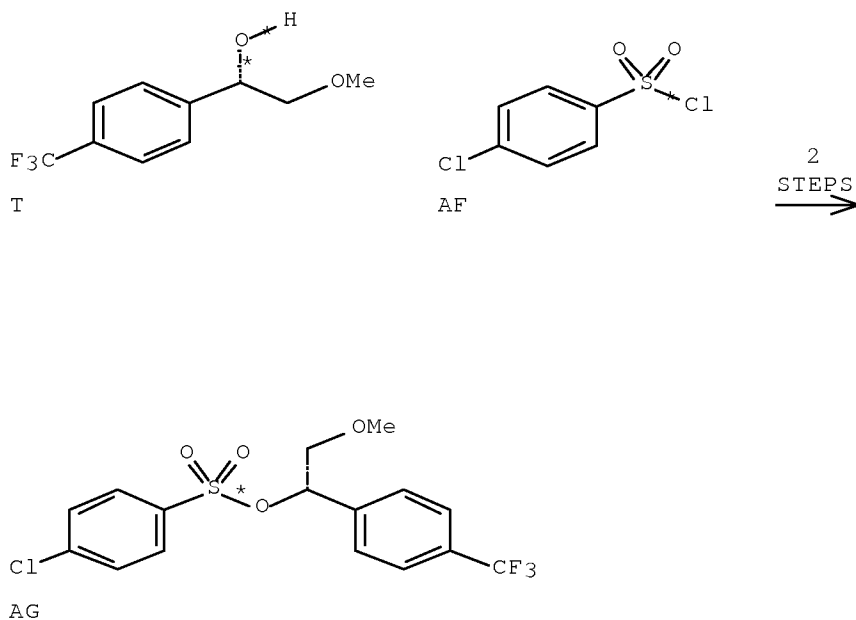


AB Chiral 1-substituted-2-methylpiperazines I [X = alkyl, halogen, haloalkyl, alkoxy, aryl, aryloxy, heteroaryl; n = 1-5; Z = alkyl, alkoxyalkyl, aryl, heteroaryl, heteroaralkyl, aralkyl] are prepared by treating 4-protected (S)-2-methylpiperazine with (S)-XnC<sub>6</sub>H<sub>4</sub>CHZO<sub>3</sub>sY [Y = alkyl, haloalkyl, (un)substituted aryl] and deblocking. Thus, 4-F<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>OMe was reduced to (S)-4-F<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>CH(OH)CH<sub>2</sub>OMe with a chiral borane and converted to (S)-4-F<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>CH(CH<sub>2</sub>OMe)O<sub>3</sub>SC<sub>6</sub>H<sub>4</sub>Cl-4 which was treated with (S)-4-benzyloxycarbonyl-2-methylpiperazine and deblocked to give I [X = 4-F<sub>3</sub>C, Z = CH<sub>2</sub>OMe].

RX(45) OF 104 COMPOSED OF REACTION SEQUENCE RX(10), RX(13)  
AND REACTION SEQUENCE RX(2), RX(13)

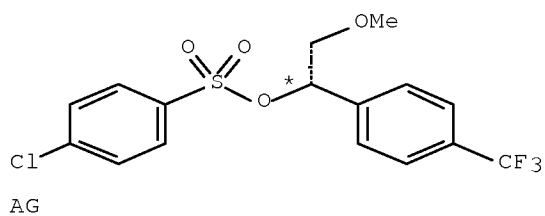
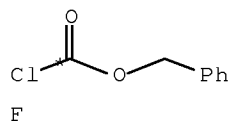
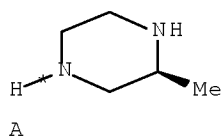
...T + AF ==> AG...

...A + F + AG ==> AM

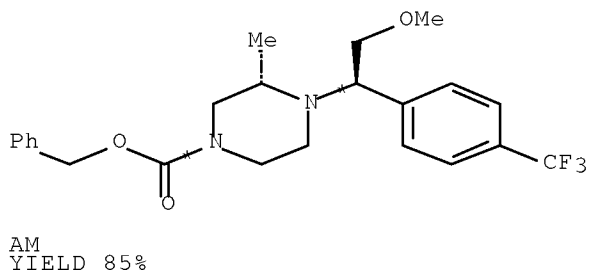


START NEXT REACTION SEQUENCE





2  
STEPS  
→



RX(10) RCT T 612493-93-3, AF 98-60-2

STAGE(1)

RGT AH 280-57-9 Triethylenediamine

SOL 108-88-3 PhMe

CON SUBSTAGE(1) 1 hour, -5 - -15 deg C

SUBSTAGE(2) 1 hour, -5 - -15 deg C

STAGE(2)

RGT J 7732-18-5 Water

PRO AG 612493-96-6

RX(2) RCT A 74879-18-8, F 501-53-1

RGT H 64-19-7 AcOH

PRO G 612493-87-5

SOL 67-56-1 MeOH, 7732-18-5 Water

CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C

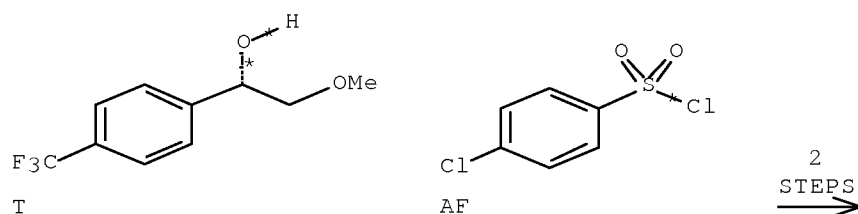
SUBSTAGE(2) 1 hour, 0 - 10 deg C

NTE regioselective

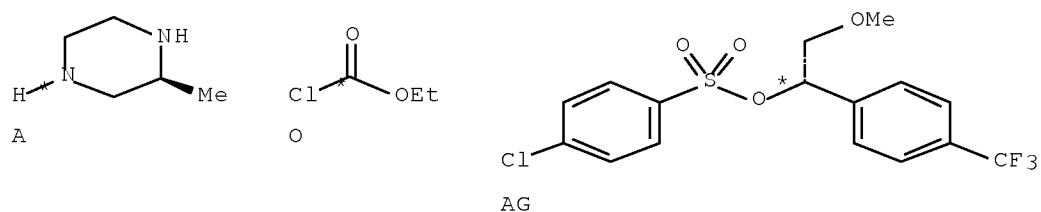
RX(13)      RCT    G 612493-87-5, AG 612493-96-6  
               RGT    D 584-08-7 K2CO3  
               PRO    AM 612494-01-6  
               SOL    108-88-3 PhMe, 75-05-8 MeCN  
               CON    SUBSTAGE(1) room temperature  
                       SUBSTAGE(2) 30 hours, 80 - 85 deg C  
               NTE    stereoselective, optimization study

RX(49) OF 104 COMPOSED OF REACTION SEQUENCE RX(10), RX(17)  
 AND REACTION SEQUENCE RX(5), RX(17)

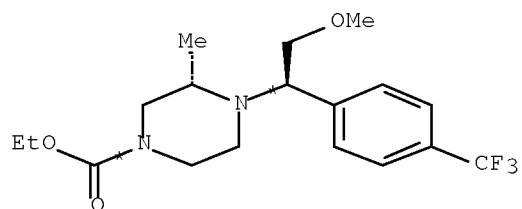
...T + AF ==> AG...  
 ...A + C + AG ==> AR



START NEXT REACTION SEQUENCE



2  
STEPS  
→



AR  
YIELD 88%

RX(10) RCT T 612493-93-3, AF 98-60-2

STAGE(1)

RGT AH 280-57-9 Triethylenediamine

SOL 108-88-3 PhMe

CON SUBSTAGE(1) 1 hour, -5 - -15 deg C

SUBSTAGE(2) 1 hour, -5 - -15 deg C

STAGE(2)

RGT J 7732-18-5 Water

PRO AG 612493-96-6

RX(5) RCT A 74879-18-8, O 541-41-3

RGT H 64-19-7 AcOH

PRO P 612493-91-1

SOL 7732-18-5 Water, 67-56-1 MeOH

CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C

SUBSTAGE(2) 1 hour, 0 - 10 deg C

NTE regioselective

RX(17) RCT P 612493-91-1, AG 612493-96-6

RGT D 584-08-7 K2CO3

PRO AR 612494-06-1

SOL 108-88-3 PhMe, 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

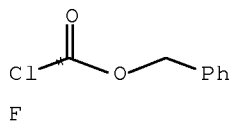
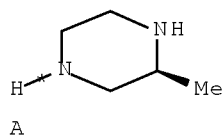
SUBSTAGE(2) 20 hours, 80 - 85 deg C

NTE stereoselective

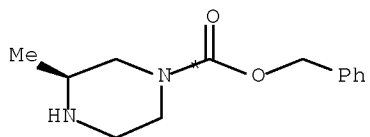
RX(73) OF 104 COMPOSED OF REACTION SEQUENCE RX(2), RX(13)  
AND REACTION SEQUENCE RX(7), RX(10), RX(13)

...A + F ==> G...

...S + AF + G ==> AM

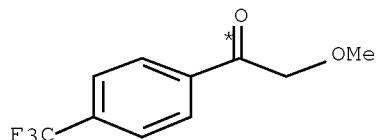


3  
STEPS  
→

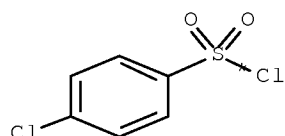


G

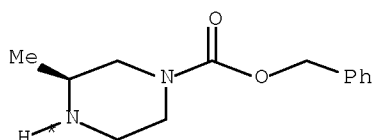
START NEXT REACTION SEQUENCE



S

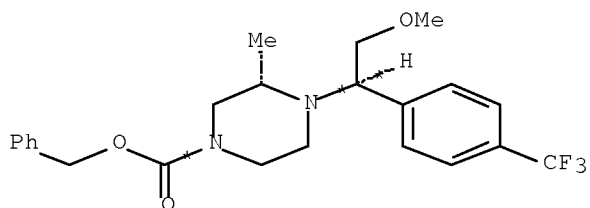


AF



G

3  
STEPS  
→



AM  
YIELD 85%

RX(2)	RCT	A 74879-18-8, F 501-53-1
	RGT	H 64-19-7 AcOH
	PRO	G 612493-87-5
	SOL	67-56-1 MeOH, 7732-18-5 Water
	CON	SUBSTAGE(1) 90 minutes, 0 - 10 deg C
		SUBSTAGE(2) 1 hour, 0 - 10 deg C
	NTE	regioselective
RX(7)	RCT	S 26771-69-7

## STAGE(1)

RGT U 75-75-2 MeSO<sub>3</sub>H, V 14044-65-6 BH<sub>3</sub>-THF  
 SOL 109-99-9 THF, 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 10 minutes, room temperature

## STAGE(2)

RGT W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,  
 tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 30 minutes, room temperature

## STAGE(3)

SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 1 hour, 20 - 30 deg C  
 SUBSTAGE(2) 1 hour, room temperature

## STAGE(4)

SOL 67-56-1 MeOH  
 CON 10 - 20 deg C

PRO T 612493-93-3  
 NTE stereoselective

RX(10) RCT T 612493-93-3, AF 98-60-2

## STAGE(1)

RGT AH ~~280-57-9~~ Triethylenediamine  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 1 hour, -5 - -15 deg C  
 SUBSTAGE(2) 1 hour, -5 - -15 deg C

## STAGE(2)

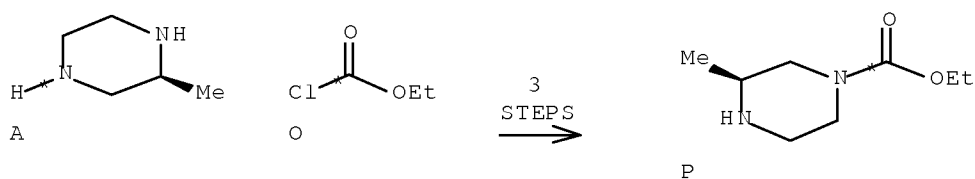
RGT J 7732-18-5 Water

PRO AG 612493-96-6

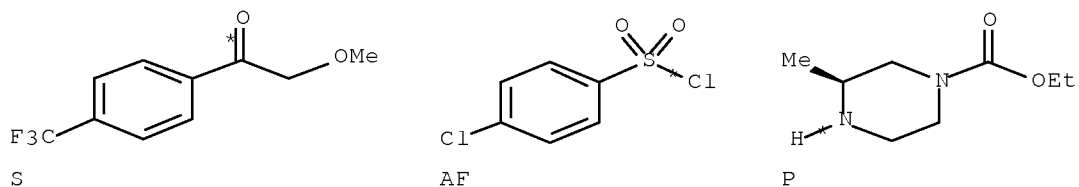
RX(13) RCT G 612493-87-5, AG 612493-96-6  
 RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO AM ~~612494-01-6~~  
 SOL 108-88-3 PhMe, 75-05-8 MeCN  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 30 hours, 80 - 85 deg C  
 NTE stereoselective, optimization study

RX(76) OF 104 COMPOSED OF REACTION SEQUENCE RX(5), RX(17)  
 AND REACTION SEQUENCE RX(7), RX(10), RX(17)

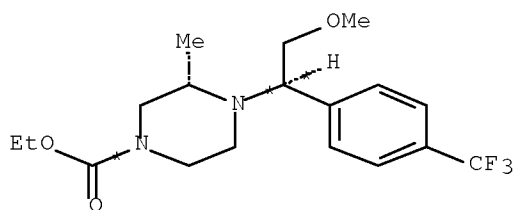
...A + O ==> P...  
 ...S + AF + P ==> AR



START NEXT REACTION SEQUENCE



3  
 STEPS



AR  
YIELD 88%

RX(5)      RCT    A 74879-18-8, O 541-41-3  
               RGT    H 64-19-7 AcOH  
               PRO    P 612493-91-1  
               SOL    7732-18-5 Water, 67-56-1 MeOH  
               CON    SUBSTAGE(1) 90 minutes, 0 - 10 deg C  
                       SUBSTAGE(2) 1 hour, 0 - 10 deg C  
               NTE    regioselective

RX(7)      RCT    S 26771-69-7

STAGE(1)

RGT    U 75-75-2 MeSO<sub>3</sub>H, V 14044-65-6 BH<sub>3</sub>-THF  
 SOL    109-99-9 THF, 108-88-3 PhMe

CON SUBSTAGE(1) room temperature  
SUBSTAGE(2) 10 minutes, room temperature

STAGE(2)

RGT W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,  
tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-

SOL 108-88-3 PhMe

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 30 minutes, room temperature

STAGE(3)

SOL 108-88-3 PhMe

CON SUBSTAGE(1) 1 hour, 20 - 30 deg C

SUBSTAGE(2) 1 hour, room temperature

STAGE(4)

SOL 67-56-1 MeOH

CON 10 - 20 deg C

PRO T 612493-93-3

NTE stereoselective

RX(10) RCT T 612493-93-3, AF 98-60-2

STAGE(1)

RGT AH 280-57-9 Triethylenediamine

SOL 108-88-3 PhMe

CON SUBSTAGE(1) 1 hour, -5 - -15 deg C

SUBSTAGE(2) 1 hour, -5 - -15 deg C

STAGE(2)

RGT J 7732-18-5 Water

PRO AG 612493-96-6

RX(17) RCT P 612493-91-1, AG 612493-96-6

RGT D 584-08-7 K2CO3

PRO AR 612494-06-1

SOL 108-88-3 PhMe, 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

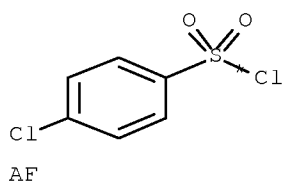
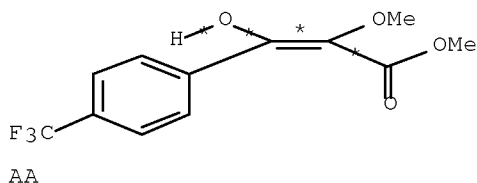
SUBSTAGE(2) 20 hours, 80 - 85 deg C

NTE stereoselective

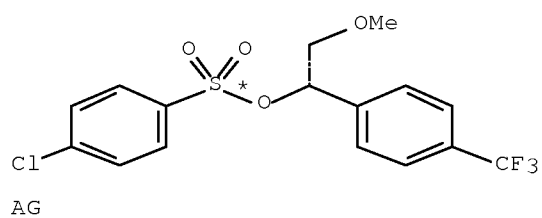
RX(82) OF 104 COMPOSED OF REACTION SEQUENCE RX(9), RX(7), RX(10), RX(13)  
AND REACTION SEQUENCE RX(2), RX(13)

...AA + AF ==> AG...

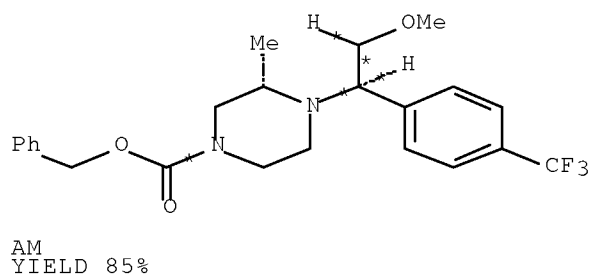
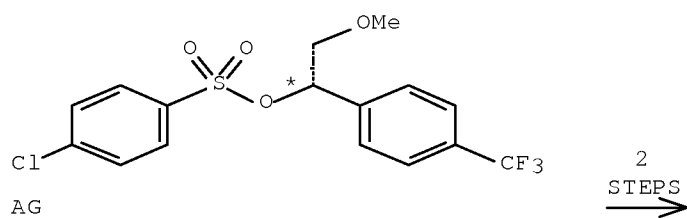
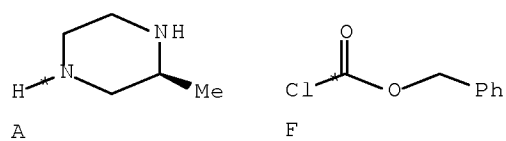
...A + F + AG ==> AM



2  
STEPS  
→



START NEXT REACTION SEQUENCE



RX(9) RCT AA 612493-95-5  
RGT AC 7664-93-9 H2SO4  
PRO S 26771-69-7  
SOL 67-56-1 MeOH, 7732-18-5 Water

RX(7) RCT S 26771-69-7



## STAGE(1)

RGT U 75-75-2 MeSO<sub>3</sub>H, V 14044-65-6 BH<sub>3</sub>-THF  
 SOL 109-99-9 THF, 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 10 minutes, room temperature

## STAGE(2)

RGT W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,  
 tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 30 minutes, room temperature

## STAGE(3)

SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 1 hour, 20 - 30 deg C  
 SUBSTAGE(2) 1 hour, room temperature

## STAGE(4)

SOL 67-56-1 MeOH  
 CON 10 - 20 deg C

PRO T 612493-93-3  
 NTE stereoselective

RX(10) RCT T 612493-93-3, AF 98-60-2

## STAGE(1)

RGT AH ~~280-57-9~~ Triethylenediamine  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 1 hour, -5 - -15 deg C  
 SUBSTAGE(2) 1 hour, -5 - -15 deg C

## STAGE(2)

RGT J 7732-18-5 Water

PRO AG 612493-96-6

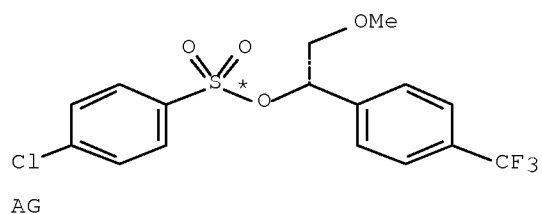
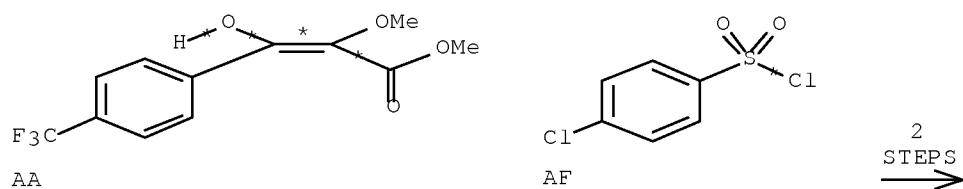
RX(2) RCT A 74879-18-8, F ~~501-53-1~~  
 RGT H 64-19-7 AcOH  
 PRO G 612493-87-5  
 SOL 67-56-1 MeOH, 7732-18-5 Water  
 CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C  
 SUBSTAGE(2) 1 hour, 0 - 10 deg C  
 NTE regioselective

RX(13) RCT G 612493-87-5, AG 612493-96-6  
 RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO AM ~~612494-01-6~~  
 SOL 108-88-3 PhMe, 75-05-8 MeCN  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 30 hours, 80 - 85 deg C  
 NTE stereoselective, optimization study

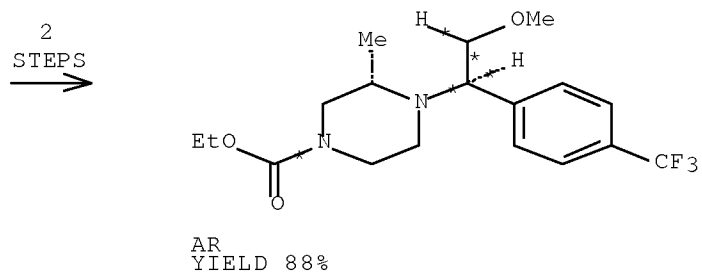
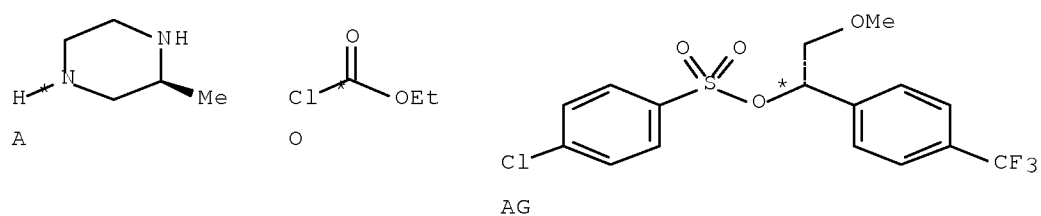
RX(87) OF 104 COMPOSED OF REACTION SEQUENCE RX(9), RX(7), RX(10), RX(17)  
 AND REACTION SEQUENCE RX(5), RX(17)

...AA + AF ==> AG...

...A + O + AG ==> AR



START NEXT REACTION SEQUENCE



RX(9)      RCT    AA 612493-95-5  
               RGT    AC 7664-93-9 H2SO4  
               PRO    S 26771-69-7  
               SOL    67-56-1 MeOH, 7732-18-5 Water

RX(7)      RCT    S 26771-69-7

## STAGE(1)

RGT U 75-75-2 MeSO<sub>3</sub>H, V 14044-65-6 BH<sub>3</sub>-THF  
 SOL 109-99-9 THF, 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 10 minutes, room temperature

## STAGE(2)

RGT W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,  
 tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 30 minutes, room temperature

## STAGE(3)

SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 1 hour, 20 - 30 deg C  
 SUBSTAGE(2) 1 hour, room temperature

## STAGE(4)

SOL 67-56-1 MeOH  
 CON 10 - 20 deg C

PRO T 612493-93-3  
 NTE stereoselective

RX(10) RCT T 612493-93-3, AF 98-60-2

## STAGE(1)

RGT AH ~~280-57-9~~ Triethylenediamine  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 1 hour, -5 - -15 deg C  
 SUBSTAGE(2) 1 hour, -5 - -15 deg C

## STAGE(2)

RGT J 7732-18-5 Water

PRO AG 612493-96-6

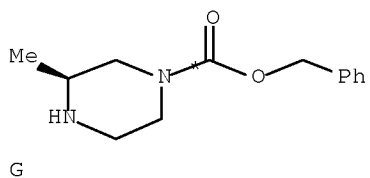
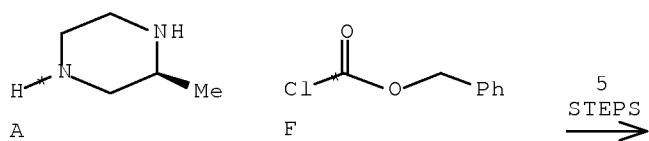
RX(5) RCT A 74879-18-8, O ~~541-41-3~~  
 RGT H 64-19-7 AcOH  
 PRO P 612493-91-1  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C  
 SUBSTAGE(2) 1 hour, 0 - 10 deg C  
 NTE regioselective

RX(17) RCT P 612493-91-1, AG 612493-96-6  
 RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO AR ~~612494-06-1~~  
 SOL 108-88-3 PhMe, 75-05-8 MeCN  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 20 hours, 80 - 85 deg C  
 NTE stereoselective

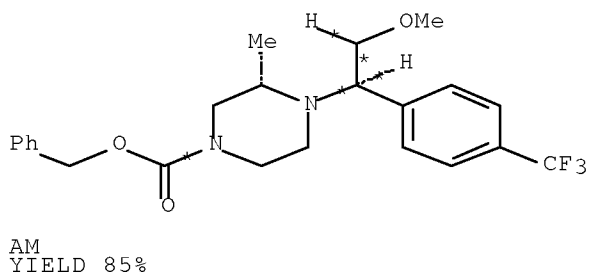
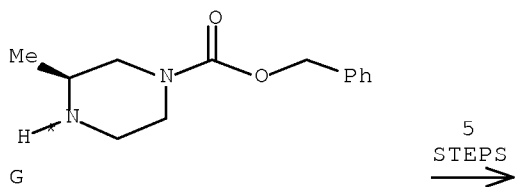
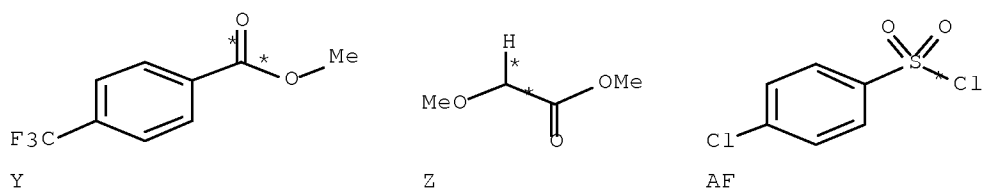
RX(91) OF 104 COMPOSED OF REACTION SEQUENCE RX(2), RX(13)  
 AND REACTION SEQUENCE RX(8), RX(9), RX(7), RX(10), RX(13)

...A + F ==> G...

...Y + Z + AF + G ==> AM



START NEXT REACTION SEQUENCE



RX(2) RCT A 74879-18-8, F 501-53-1  
 RGT H 64-19-7 AcOH  
 PRO G 612493-87-5  
 SOL 67-56-1 MeOH, 7732-18-5 Water  
 CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C  
 SUBSTAGE(2) 1 hour, 0 - 10 deg C  
 NTE regioselective

RX(8) RCT Y 2967-66-0, Z 6290-49-9  
  
 STAGE(1)  
 RGT AB 124-41-4 NaOMe  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) 5 hours, -10 deg C  
 SUBSTAGE(2) 21 hours, -10 deg C  
  
 STAGE(2)  
 RGT AC 7664-93-9 H2SO4  
 SOL 7732-18-5 Water, 1634-04-4 t-BuOMe  
 CON -8.5 deg C  
  
 PRO AA 612493-95-5  
 NTE combined yield of 82%

RX(9) RCT AA 612493-95-5  
 RGT AC 7664-93-9 H2SO4  
 PRO S 26771-69-7  
 SOL 67-56-1 MeOH, 7732-18-5 Water

RX(7) RCT S 26771-69-7  
  
 STAGE(1)  
 RGT U 75-75-2 MeSO3H, V 14044-65-6 BH3-THF  
 SOL 109-99-9 THF, 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 10 minutes, room temperature  
  
 STAGE(2)  
 RGT W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,  
 tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 30 minutes, room temperature  
  
 STAGE(3)  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 1 hour, 20 - 30 deg C  
 SUBSTAGE(2) 1 hour, room temperature  
  
 STAGE(4)  
 SOL 67-56-1 MeOH  
 CON 10 - 20 deg C  
  
 PRO T 612493-93-3  
 NTE stereoselective

RX(10) RCT T 612493-93-3, AF 98-60-2

STAGE(1)

RGT AH 280-57-9 Triethylenediamine

SOL 108-88-3 PhMe

CON SUBSTAGE(1) 1 hour, -5 - -15 deg C

SUBSTAGE(2) 1 hour, -5 - -15 deg C

STAGE(2)

RGT J 7732-18-5 Water

PRO AG 612493-96-6

RX(13) RCT G 612493-87-5, AG 612493-96-6

RGT D 584-08-7 K<sub>2</sub>CO<sub>3</sub>

PRO AM 612494-01-6

SOL 108-88-3 PhMe, 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 30 hours, 80 - 85 deg C

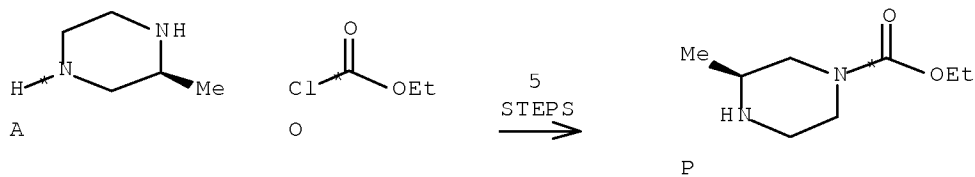
NTE stereoselective, optimization study

RX(94) OF 104 COMPOSED OF REACTION SEQUENCE RX(5), RX(17)

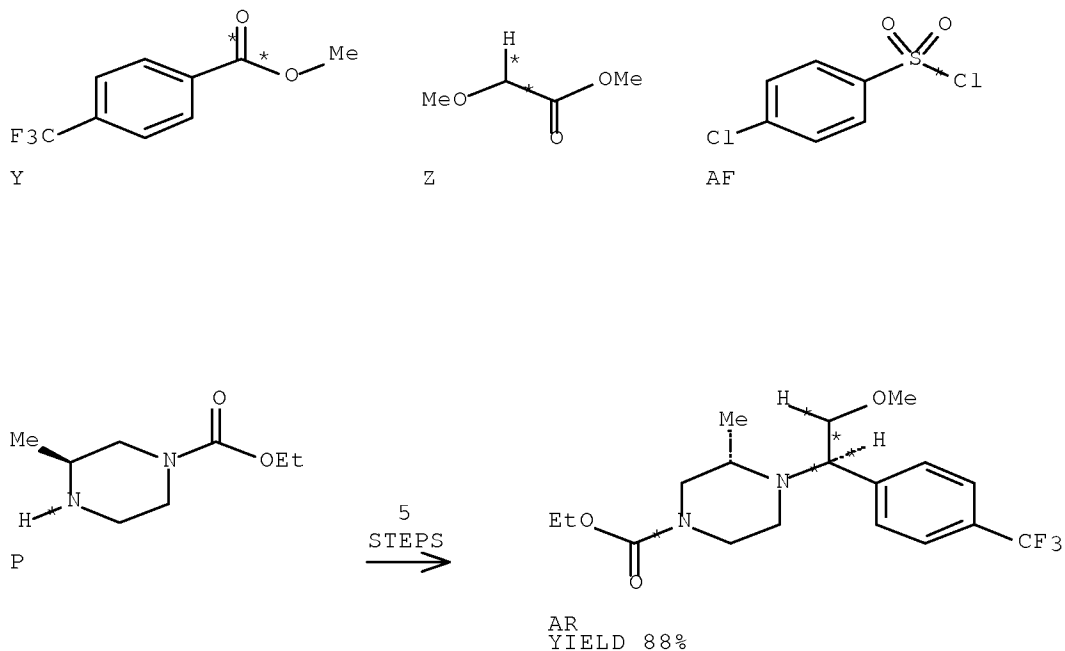
AND REACTION SEQUENCE RX(8), RX(9), RX(7), RX(10), RX(17)

...A + Q ==> P...

...Y + Z + AF + P ==> AR



START NEXT REACTION SEQUENCE



RX(5) RCT A 74879-18-8, O 541-41-3  
 RGT H 64-19-7 AcOH  
 PRO P 612493-91-1  
 SOL 7732-18-5 Water, 67-56-1 MeOH  
 CON SUBSTAGE(1) 90 minutes, 0 - 10 deg C  
 SUBSTAGE(2) 1 hour, 0 - 10 deg C  
 NTE regioselective

RX(8) RCT Y 2967-66-0, Z 6290-49-9  
  
 STAGE(1)  
 RGT AB 124-41-4 NaOMe  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) 5 hours, -10 deg C  
 SUBSTAGE(2) 21 hours, -10 deg C  
  
 STAGE(2)  
 RGT AC 7664-93-9 H2SO4  
 SOL 7732-18-5 Water, 1634-04-4 t-BuOMe  
 CON -8.5 deg C  
  
 PRO AA 612493-95-5  
 NTE combined yield of 82%

RX(9) RCT AA 612493-95-5  
 RGT AC 7664-93-9 H2SO4  
 PRO S 26771-69-7  
 SOL 67-56-1 MeOH, 7732-18-5 Water

RX(7) RCT S 26771-69-7  
  
 STAGE(1)  
 RGT U 75-75-2 MeSO3H, V 14044-65-6 BH3-THF  
 SOL 109-99-9 THF, 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 10 minutes, room temperature  
  
 STAGE(2)  
 RGT W 112022-81-8 1H,3H-Pyrrolo[1,2-c][1,3,2]oxazaborole,  
 tetrahydro-1-methyl-3,3-diphenyl-, (3aS)-  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 30 minutes, room temperature  
  
 STAGE(3)  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 1 hour, 20 - 30 deg C  
 SUBSTAGE(2) 1 hour, room temperature  
  
 STAGE(4)  
 SOL 67-56-1 MeOH  
 CON 10 - 20 deg C  
  
 PRO T 612493-93-3  
 NTE stereoselective

RX(10) RCT T 612493-93-3, AF 98-60-2

STAGE(1)

RGT AH 280-57-9 Triethylenediamine

SOL 108-88-3 PhMe

CON SUBSTAGE(1) 1 hour, -5 - -15 deg C

SUBSTAGE(2) 1 hour, -5 - -15 deg C

STAGE(2)

RGT J 7732-18-5 Water

PRO AG 612493-96-6

RX(17) RCT P 612493-91-1, AG 612493-96-6

RGT D 584-08-7 K2CO3

PRO AR 612494-06-1

SOL 108-88-3 PhMe, 75-05-8 MeCN

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 20 hours, 80 - 85 deg C

NTE stereoselective

=> d his

(FILE 'HOME' ENTERED AT 11:52:01 ON 01 FEB 2008)

FILE 'REGISTRY' ENTERED AT 11:52:06 ON 01 FEB 2008

FILE 'CASREACT' ENTERED AT 11:52:10 ON 01 FEB 2008

L1 STRUCTURE UPLOADED

L2 2 S L1 FULL

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

132.70

133.37

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-1.50

-1.50

STN INTERNATIONAL LOGOFF AT 11:53:55 ON 01 FEB 2008